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NUMERICAL SIMULATION OF THERMOLUMINESCENCE DOSE RESPONSE OF QUARTZ

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Abstract: In the current work, it has been presented TL model, which includes one trap three recombination centers. Simulation of the model followed the stages of irradiation, relaxation, and heating. The appropriate set of coupled differential equations has been developed for each stage. Numerical solving of those equations in sequence it has been demonstrated that, with appropriate choices of the sets of trapping parameters, three TL peaks occur related to three recombination centers. Thus, we can conclude that they would have different emission spectra.

Key words: numerical simulation; thermoluminescence; irradiation

1. Introduction

Thermoluminescence (TL) emission of light might be considered as delayed phosphorescence, based on the metastable accumulation of electrons and holes in defects of quartz or other crystalline insulators due to ionizing radiation and the recombination of a certain amount of them after their release by phonons upon heating. Variation of TL signal intensity as a function of absorbed dose for a given set of conditions (dose rate, material, etc.) may be termed its dose response curve. A variety of forms of dose response curves have been categorized as linear, superlinear, sublinear, and supralinear [1]. In TL dating, the choice of the mathematical function used for obtaining the equivalent dose value (D_E) through the fitting of the dose response data points is crucial because of its direct influence on the D_E value. This function should fulfill at least two fundamental criteria: it should have a physical justification and fit the experimental points. To describe the experimental data, polynomial or linear approximations have been made at low doses and saturating exponential fits at moderate doses. The application of a single saturating exponential (SSE) function is based on the assumption that the TL signal is generated by a single electron trap. A broadly applicable function for describing luminescence dose response has been developed to account for the appearance of linear, superlinear, sublinear, and supralinear behaviors and variations in saturating signal level and rate [2]. TL can be understood by considering the simplest model consisting of two localized energetic levels an isolated electron trap and a recombination center. This is commonly referred to as "**o**ne **t**rap **o**ne **r**ecombination" (OTOR) center model demonstrating the basics of the TL phenomena in general. OTOR model enables us to derive fundamental expressions for the first-, second- and general-order TL kinetics but fails to describe linear, superlinear, sublinear, and supralinear dose response and dose rate dependency. Using rather simple models of trapping states and recombination centers it has been demonstrated by [3] a dose rate dependency of trap filling. Chen and Leung [2] demonstrated that the dose rate effect seen in experiments is consistent with the basic models of trapping, detrapping, and recombination using reasonable values for the physical parameters. They included two types of recombination centers and one trapping (OTTR) state in the model, including the stages of irradiation, relaxation, and heating, covering the entire TL cycle. The main task in this work is to develop the model,

which demonstrates the origin of three components in the emission of TL in quartz, namely, UV, blue and, green.

One trap three recombination center model

In typical TL experiments, the sample goes through three stages: irradiation, relaxation, and heating. During the first stage, the irradiation produces free electrons (e^-) and holes (h^+) at the rate of G(e,h)*J, where G(e) and G(h) are the radiation chemical yield of electrons and holes respectively; J is the dose rate. Figure 1 depicts the major features of the suggested one trap three recombination center (OTThR) model. V1, V2, V3 are the three recombination centers, with the given concentrations of V1, V2, and V3 of these centers. v1, v2 and v3, are the instantaneous concentrations of holes in these centers respectively.

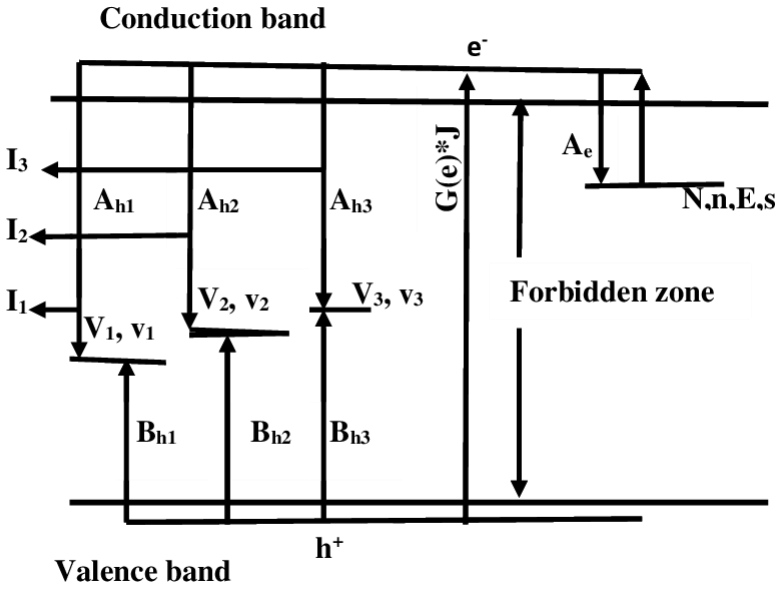

Fig. 1. One trap three recombination center model for the thermoluminescence process. The transitions take place during the irradiation and the heating of the sample is indicated by arrows. The meaning of the different parameters and the values chosen for them are given in the text.

B_{h1}, B_{h2}, and B_{h3} are the probabilities of capturing holes in V_1, V_2, and V_3, respectively, whereas Ah1, Ah2, and Ah3 are, respectively, the three recombination probabilities of free electrons with captured holes. It is worth to note that, recombination of these particles take place both during the irradiation stage and during the heating of the sample. During the heating, the stage sample is heated with a linear heating rate β=dT/dt from 50°C up to a high temperature usually around 500°C. The electrons trapped during the irradiation stage are thermally released from the level N into the conduction band, as the temperature of the sample is increased. N stands for the total concentration of electron trapping states, n is the instantaneous concentration of occupied traps. The number of recombination centers, V1, V2, and V3, and also the number of electron trapping states, N remain constant during the full cycle of TL experiment e.g. irradiation, relaxation, and heating. E and s are the activation energy and frequency factor of the electron trap, respectively. A_{e-} is the trapping (retrapping during heating) probability of electrons from the conduction band. According to the described schema in Fig.1, the set of differential equations governing the process during the irradiation stage is

$$\frac{dh^+}{dt} = G(e) * J - B_{h1}([V_1] - [v_1])[h^+] - B_{h2}([V_2] - [v_2])[h^+] \quad (1)$$

$$\frac{d\,v_1}{dt} = -A_{v1}[v_1][e] + B_{h1}([V_1] - [v_1])[h^+] \quad (2)$$

$$\frac{d\,v_2}{dt} = -A_{v2}[v_2][e] + B_{h2}([V_2] - [v_2])[h^+] \quad (3)$$

$$\frac{d\,v_3}{dt} = -A_{v3}[v_3][e] + B_{h3}([V_3] - [v_3])[h^+] \quad (4)$$

$$\frac{d\,n}{dt} = A_e([N] - [n]) * [e] \quad (5)$$

$$\frac{d\,e^-}{dt} = \frac{d\,v_1}{dt} + \frac{d\,v_2}{dt} + \frac{d\,v_3}{dt} + \frac{dh^+}{dt} - \frac{d\,n}{dt} \quad (6)$$

This is followed by a relaxation stage. The generation of electrons and holes does not occur either at this stage or at the next stage of heating, which means that G (e-, h +) * J = 0, therefore [h+] will also be zero. Hence B_{h1}, B_{h2}, and B_{h3} are irrelevant during this stage. As for free electrons, they may be thermally released from trapped states N, into the conduction band, and then either retrap or recombine with holes in V_1, V_2, and V_3, respectively.

1) thermal release;
2) retrapping of free electrons by electron trapping states;
3) recombination with holes in V_1, V_2, and V_3.

Reactions described above lead to the following set of differential equations:

$$\frac{d\,v_1}{dt} = -A_{v1}[v_1][e] \quad (7)$$

$$\frac{d\,v_2}{dt} = -A_{v2}[v_2][e] \quad (8)$$

$$\frac{d\,v_3}{dt} = -A_{v3}[v_3][e] \quad (9)$$

$$\frac{d\,n}{dt} = -snexp(^{-E}/_{kT}) + A_e([N] - [n]) * [e] \quad (10)$$

$$\frac{d\,e^-}{dt} = \frac{d\,v_1}{dt} + \frac{d\,v_2}{dt} + \frac{d\,v_3}{dt} - \frac{d\,n}{dt} \quad (11)$$

The same MatLab ode45 solver was used to solve the set of equations describing the heating stage. To solve them with the temperature change it has been used new independent parameter, namely the temperature changing linearly with a constant heating rate β:

$$\frac{dy}{dt} = \frac{dy}{dt}\frac{dt}{dT} \text{ and } T=T_0+\beta t$$

OTThR model does not consider non-irradiative recombination centers and all three recombination centers are radiative. Thus, the intensity of each TL glow curves is proportional to the rate of changes of v1, v2, v3, i.e.

$$I_{m1}(T) = -dv_1 / dt \quad (12)$$

$$I_{m2}(T) = -dv_2 / dt \quad (13)$$

$$I_{m3}(T) = -dv_3 / dt \quad (14)$$

2. Results and Discussions

For the given set trapping parameters equations of (1)-(6) were numerically soled using the ode45 solver in the MatLab package, for the time of irradiation t, Thus, the total dose of irradiation

is J*t. Numerical solution of differential equations depends on chosen initial parameters. We have looked for different plausible parameters and the following set of parameters were tested. As a criterion it was taken the parameters for the one trap two recombination center model [2], in order to have comparable results. The following set of parameters was found to produce the results which are in line with the experimental data: E=1.38eV; s=1e+10 s^{-1}; A_{v1}= 1e-18 m^3/s; A_{v2}= 1e-19 m^3/s; A_{v3}= 2e-19 m^3/s; V_{h1}=1e-19 m^3/s; V_{h2}=1.5e-19 m^3/s; V_{h3}=1e-19 m^3/s; A_{e-}=1e-20; N=1e+20 m^{-3}; V_1=1e+20 m^{-3}; V_2=1e+20 m^{-3}; V_3=1e+20 m^{-3};

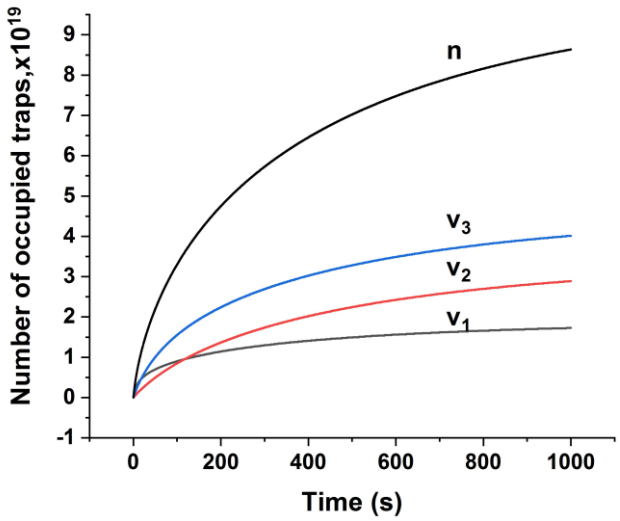

Fig. 2. Kinetics of accumulation of trapped holes and electrons during the irradiation stage. v_1, v_2, and v_3 are the concentrations trapped holes, and n stands for the trapped electrons.

Fig.2 illustrates the result of the solution of the equations related to the irradiation stage, i.e. from (1) to (6) with the set of above-mentioned parameters and G(e^-)*J=1e+18 m^3/s and irradiation time of 1e+3 s. The initial concentrations of all six variables (e-, h+, v_1, v_2, v_3, and n) have been taken equal to zero. After the simulation we are getting certain values of the trapped electrons and holes.

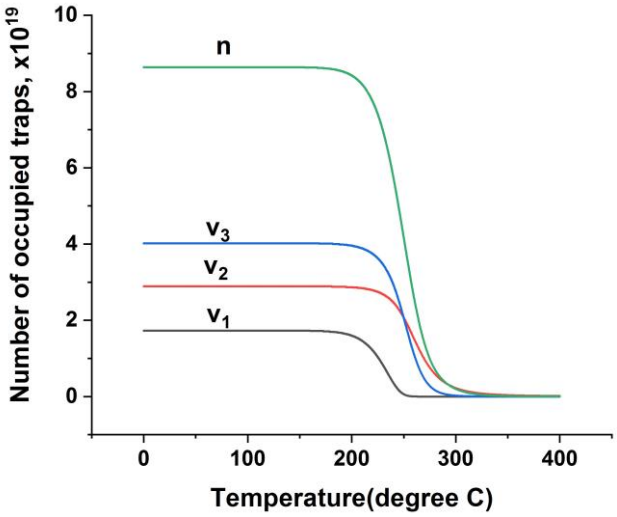

Fig. 3. Kinetics of accumulation of trapped holes and electrons during the heating stage. v_1, v_2, and v_3 are the concentrations trapped holes, and n stands for the trapped electrons.

This is followed by the relaxation stage and it is obvious that no electron or hole production takes place, which means that during this stage as well as during heating stage $G(e^-,h^+)*J= 0$. Simulation of relaxation stage for approximately ten seconds results in decreasing of concentration of holes to zero, the concentration of free electrons close to zero, and flat concentration of trapped holes and electrons. For the sake of simplicity, the results of the relaxation stage have not been illustrated here. The results of the simulation for the relaxation stage have been considered as initial conditions for the heating stage: eq. from (7) to (11) and illustrated in Fig.3.

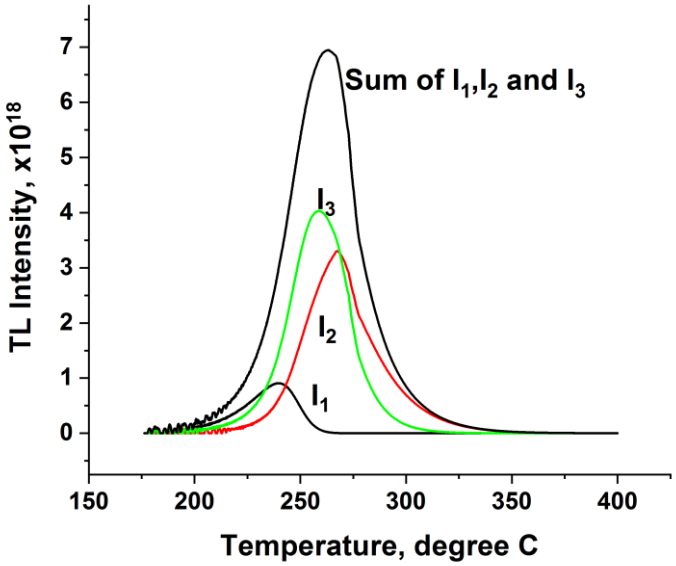

Fig. 4. Three TL peaks (I_1, I_2,and I_3) as calculated with the model of three recombination centers and one trapping state. They might be attributed to three components in the emission of TL in quartz, namely, UV, blue, and green. The set of parameters applied is given in the text. The sum of peaks is attributed to the total TL peak.

Fig.4 illustrates the height and the temperature at the peak maximum depending on the chosen initial conditions. Therefore, the height and temperature at the maximum of the total peak (sum of peaks I_1, I_2, and I_3) can also depend on the values of its constituents. This, in turn, means that the parameters of the recombination centers and electronic states strongly influence the shape of the dose-dependence curve which often has been reported in the literature.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ТЕРМОЛЮМИНЕСЦЕНТНОЙ ЭМИССИИ КВАРЦА В ЗАВИСИМОСТИ ОТ ДОЗЫ ОБЛУЧЕНИЯ

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Резюме: В данной работе была представлена модель TL, включающая одну ловушку и три рекомбинационных центра. Симуляция модели сопровождалось этапами облучения, релаксации и нагрева. Соответствующий набор связанных дифференциальных уравнений был разработан для каждой стадии. Численное решение этих уравнений в последовательности продемонстрировало, что при соответствующем выборе наборов параметров захвата возникают три пика TL, связанных с тремя центрами рекомбинации. Таким образом, можно сделать вывод, что они будут иметь разные спектры излучения.

Ключевые слова*: цифровая симуляция; термолюминесценция; облучения*

ŞÜALANMIŞ KVARSIN TERMOLÜMİNESSENSİYA EMİSSİYASININ RİYAZİ MODELLƏŞDİRİLMƏSİ

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Xülasə: Bu məqalədə, bir tələ və üç rekombinasiya mərkəzi də daxil olmaqla TL modeli təqdim edildi. Modelin simulyasiyası üç mərhələdən: şüalanma, relaksasiya və qızdırılma mərhələlərindən ibarət olmuşdur. Hər mərhələ üçün uyğun diferensial tənliklər sistemi hazırlanmışdır. Bu tənliklərin ardıcıllıqla həll edilməsi göstərdi ki, ilkin parametrlər dəstinin müvafiq seçimi ilə üç rekombinasiya mərkəzi ilə əlaqəli üç TL piki meydana gəlir. Beləliklə, onların fərqli emissiya spektrlərinin olacağına dair nəticəyə gələ bilərik.

Açar sözlər: rəqəmsal simulyasiya; termoluminessensiyaı; şüalanma